Eliseo Ruiz

List of Publications by Citations

276 papers	15,532 citations	66 h-index	115 g-index
288 ext. papers	16,410 ext. citations	6.1 avg, IF	6.64 L-index

#	Paper	IF	Citations
276	Broken symmetry approach to calculation of exchange coupling constants for homobinuclear and heterobinuclear transition metal complexes **1999**, 20, 1391-1400		779
275	Toward the Prediction of Magnetic Coupling in Molecular Systems: Hydroxo- and Alkoxo-Bridged Cu(II) Binuclear Complexes. *Journal of the American Chemical Society*, **1997**, 119, 1297-1303	16.4	773
274	Magnetic Coupling in End-On Azido-Bridged Transition Metal Complexes: A Density Functional Study. *Journal of the American Chemical Society*, **1998**, 120, 11122-11129	16.4	633
273	About the calculation of exchange coupling constants in polynuclear transition metal complexes. *Journal of Computational Chemistry*, **2003**, 24, 982-9	3.5	442
272	Structural Modeling and Magneto-Structural Correlations for Hydroxo-Bridged Copper(II) Binuclear Complexes. *Inorganic Chemistry*, **1997**, 36, 3683-3688	5.1	364
271	Mononuclear single-molecule magnets: tailoring the magnetic anisotropy of first-row transition-metal complexes. *Journal of the American Chemical Society*, **2013**, 135, 7010-8	16.4	335
270	Exchange coupling in carboxylato-bridged dinuclear copper(II) compounds: a density functional study. *Chemistry - A European Journal*, **2001**, 7, 627-37	4.8	315
269	About the calculation of exchange coupling constants using density-functional theory: the role of the self-interaction error. *Journal of Chemical Physics*, **2005**, 123, 164110	3.9	299
268	Origin of slow magnetic relaxation in Kramers ions with non-uniaxial anisotropy. *Nature Communications*, **2014**, 5, 4300	17.4	283
267	Large magnetic anisotropy in mononuclear metal complexes. *Coordination Chemistry Reviews*, **2015**, 289-290, 379-392	23.2	280
266	Slow magnetic relaxation in a Co(II)-Y(III) single-ion magnet with positive axial zero-field splitting. *Angewandte Chemie - International Edition*, **2013**, 52, 9130-4	16.4	242
265	Dual aperture control on pH- and anion-driven supramolecular nanoscopic hybrid gate-like ensembles. *Journal of the American Chemical Society*, **2008**, 130, 1903-17	16.4	209
264	Exchange coupling of transition-metal ions through hydrogen bonding: a theoretical investigation. *Journal of the American Chemical Society*, **2002**, 124, 5197-205	16.4	190
263	Field and dilution effects on the slow relaxation of a luminescent DyO9 low-symmetry single-ion magnet. *Chemical Communications*, **2012**, 48, 7916-8	5.8	189
262	Exchange Coupling in Oxalato-Bridged Copper(II) Binuclear Compounds: A Density Functional Study. *Chemistry - A European Journal*, **1998**, 4, 476-484	4.8	185
261	Can large magnetic anisotropy and high spin really coexist?. *Chemical Communications*, **2008**, 52-4	5.8	184
260	Spin Density Distribution in Transition Metal Complexes: Some Thoughts and Hints. *Comments on Inorganic Chemistry*, **1998**, 20, 27-56	3.9	180

259	Charge-Transfer Complexes: Stringent Tests for Widely Used Density Functionals. *The Journal of Physical Chemistry*, **1996**, 100, 12265-12276		176
258	Shedding light on the single-molecule magnet behavior of mononuclear Dy(III) complexes. *Inorganic Chemistry*, **2013**, 52, 13770-8	5.1	159
257	Theoretical Study of the Exchange Coupling in Large Polynuclear Transition Metal Complexes Using DFT Methods. *Structure and Bonding*, **2004**, 71-102	0.9	159
256	Asymmetric azido-copper(II) bridges: ferro- or antiferromagnetic? experimental and theoretical magneto-structural studies. *Inorganic Chemistry*, **2005**, 44, 5501-8	5.1	157
255	Spin density distribution in transition metal complexes. *Coordination Chemistry Reviews*, **2005**, 249, 2649-2660	23.6	153
254	Theoretical study of exchange coupling in 3d-Gd complexes: large magnetocaloric effect systems. *Journal of the American Chemical Society*, **2012**, 134, 10532-42	16.4	144
253	Structural and electronic effects on the exchange interactions in dinuclear bis(phenoxo)-bridged copper(II) complexes. *Coordination Chemistry Reviews*, **2010**, 254, 2086-2095	23.2	142
252	Magnetic coupling in end-to-end azido-bridged copper and nickel binuclear complexes: a theoretical study. *Inorganic Chemistry*, **2000**, 39, 3221-9	5.1	140
251	How to build molecules with large magnetic anisotropy. *Chemistry - A European Journal*, **2009**, 15, 4078-87	4.8	139
250	Electronic structure and properties of Cu2O. *Physical Review B*, **1997**, 56, 7189-7196	3.3	131
249	Shape and spin state in four-coordinate transition-metal complexes: the case of the d(6) configuration. *Chemistry - A European Journal*, **2006**, 12, 3162-7	4.8	131
248	Defining the Domain of Density Functionals: Charge-Transfer Complexes. *Journal of the American Chemical Society*, **1995**, 117, 1141-1142	16.4	130
247	Calculation of exchange coupling constants in solid state transition metal compounds using localized atomic orbital basis sets. *Journal of Solid State Chemistry*, **2003**, 176, 400-411	3.3	128
246	Family of carboxylate- and nitrate-diphenoxo triply bridged dinuclear Ni(II)Ln(III) complexes (Ln = Eu, Gd, Tb, Ho, Er, Y): synthesis, experimental and theoretical magneto-structural studies, and single-molecule magnet behavior. *Inorganic Chemistry*, **2012**, 51, 5857-68	5.1	126
245	Coherent transport through spin-crossover single molecules. *Journal of the American Chemical Society*, **2012**, 134, 777-9	16.4	123
244	Is it possible to get high T(C) magnets with Prussian blue analogues? A theoretical prospect. *Chemistry - A European Journal*, **2005**, 11, 2135-44	4.8	123
243	Electronic structure and properties of AlN. *Physical Review B*, **1994**, 49, 7115-7123	3.3	123
242	Large Conductance Switching in a Single-Molecule Device through Room Temperature Spin-Dependent Transport. *Nano Letters*, **2016**, 16, 218-26	11.5	118

241	Exchange coupling in halo-bridged dinuclear Cu(II) compounds: a density functional study. *Inorganic Chemistry*, **2002**, 41, 3769-78	5.1	114
240	Density functional study of magnetostructural correlations in cubane complexes containing the Cu4O4 core. *Journal of Materials Chemistry*, **2006**, 16, 2729-2735		100
239	Continuous Shape Measures as a Stereochemical Tool in Organometallic Chemistry. *Organometallics*, **2005**, 24, 1556-1562	3.8	99
238	Exchange coupling in transition-metal complexes via density-functional theory: comparison and reliability of different basis set approaches. *Journal of Chemical Physics*, **2005**, 123, 074102	3.9	98
237	Enhanced bistability by guest inclusion in Fe(II) spin crossover porous coordination polymers. *Chemical Communications*, **2012**, 48, 4686-8	5.8	95
236	Charge transport properties of spin crossover systems. *Physical Chemistry Chemical Physics*, **2014**, 16, 14-22	3.6	92
235	Magnetic structure of the large-spin Mn10 and Mn19 complexes: a theoretical complement to an experimental milestone. *Journal of the American Chemical Society*, **2008**, 130, 7420-6	16.4	90
234	Magnetostructural correlations in polynuclear complexes: the Fe4 butterflies. *Journal of the American Chemical Society*, **2006**, 128, 15722-7	16.4	88
233	A Low Spin Manganese(IV) Nitride Single Molecule Magnet. *Chemical Science*, **2016**, 7, 6132-6140	9.4	87
232	Equilibria between metallosupramolecular squares and triangles with the new rigid linker 1,4-bis(4-pyridyl)tetrafluorobenzene. Experimental and theoretical study of the structural dependence of NMR data. *Inorganic Chemistry*, **2003**, 42, 5890-9	5.1	87
231	Density functional study of the exchange coupling in distorted cubane complexes containing the Cu4O4 core. *Polyhedron*, **2001**, 20, 1323-1327	2.7	87
230	Rational electrostatic design of easy-axis magnetic anisotropy in a Zn(II) -Dy(III) -Zn(II) single-molecule magnet with a high energy barrier. *Chemistry - A European Journal*, **2014**, 20, 14262-9	4.8	84
229	Electronic Structure and Bonding in CuMO2 (M = Al, Ga, Y) Delafossite-Type Oxides: An Ab Initio Study. *Journal of Physical Chemistry B*, **1999**, 103, 8060-8066	3.4	83
228	Stereochemistry and spin state in four-coordinate transition metal compounds. *Inorganic Chemistry*, **2008**, 47, 2871-89	5.1	82
227	Cu(II)-Gd(III) cryogenic magnetic refrigerants and Cu8Dy9 single-molecule magnet generated by in situ reactions of picolinaldehyde and acetylpyridine: experimental and theoretical study. *Chemistry - A European Journal*, **2013**, 19, 17567-77	4.8	80
226	Benchmarking Density Functional Methods for Calculation of State Energies of First Row Spin-Crossover Molecules. *Inorganic Chemistry*, **2018**, 57, 14097-14105	5.1	77
225	Self-assembly reactions between the cis-protected metal corners (N-N)MII (N-N = ethylenediamine, 4,4'-substituted 2,2'-bipyridine; M = Pd, Pt) and the fluorinated edge 1,4-bis(4-pyridyl)tetrafluorobenzene. *Inorganic Chemistry*, **2007**, 46, 3395-406	5.1	76
224	[Cu3(mu-S)2]3+ clusters supported by N-donor ligands: progress toward a synthetic model of the catalytic site of nitrous oxide reductase. *Journal of the American Chemical Society*, **2005**, 127, 13752-3	16.4	76

223	Theoretical study of the magnetic behavior of hexanuclear Cu(II) and Ni(II) polysiloxanolato complexes. *Journal of the American Chemical Society*, **2003**, 125, 6791-4	16.4	75
222	Determining and extending the domain of exchange and correlation functionals. *International Journal of Quantum Chemistry*, **1995**, 56, 61-78	2.1	75
221	Color and Conductivity in Cu2O and CuAlO2: A Theoretical Analysis of d10□□d10 Interactions in Solid-State Compounds. *Chemistry of Materials*, **2001**, 13, 338-344	9.6	74
220	Borate-driven gatelike scaffolding using mesoporous materials functionalised with saccharides. *Chemistry - A European Journal*, **2009**, 15, 6877-88	4.8	73
219	Exchange coupling in cyano-bridged homodinuclear Cu(II) and Ni(II) complexes: synthesis, structure, magnetism, and density functional theoretical study. *Inorganic Chemistry*, **2001**, 40, 5868-77	5.1	72
218	Helical self-organization and hierarchical self-assembly of an oligoheterocyclic pyridine-pyridazine strand into extended supramolecular fibers. *Chemistry - A European Journal*, **2002**, 8, 3448-57	4.8	70
217	Synthesis, crystal structure and magnetic properties of three unprecedented tri-nuclear and one very rare tetra-nuclear copper(II) Schiff-base complexes supported by mixed azido/phenoxo/nitrato or acetato bridges. *Dalton Transactions*, **2010**, 39, 7474-84	4.3	69
216	Novel CuIII bis-1,2-dichalcogenene complexes with tunable 3D framework through alkaline cation coordination: a structural and theoretical study. *Chemistry - A European Journal*, **2004**, 10, 1691-704	4.8	69
215	Relaxation Dynamics of Identical Trigonal Bipyramidal Cobalt Molecules with Different Local Symmetries and Packing Arrangements: Magnetostructural Correlations and ab inito Calculations. *Journal of the American Chemical Society*, **2016**, 138, 16407-16416	16.4	68
214	Theoretical methods enlighten magnetic properties of a family of Mn(6) single-molecule magnets. *Inorganic Chemistry*, **2009**, 48, 8012-9	5.1	67
213	Ferromagnetic coupling in trinuclear, partial cubane Cu(II) complexes with a micro(3)-OH core: magnetostructural correlations. *Chemistry - A European Journal*, **2007**, 13, 9297-309	4.8	67
212	Ferromagnetic coupling in a 1D coordination polymer containing a symmetric [Cu(mu1,1-N3)2Cu(mu1,1-N3)2Cu]2+ core and based on an organic ligand obtained from the solid state. *Inorganic Chemistry*, **2007**, 46, 8843-50	5.1	67
211	Unexpected ferromagnetic interaction in a new tetranuclear copper(II) complex: synthesis, crystal structure, magnetic properties, and theoretical studies. *Inorganic Chemistry*, **2005**, 44, 5011-20	5.1	66
210	Symmetry and topology determine the MoV-CN-MnII exchange interactions in high-spin molecules. *Angewandte Chemie - International Edition*, **2005**, 44, 2711-2715	16.4	65
209	On the origin of ferromagnetism in oximato-based [Mn3O]7+ triangles. *Dalton Transactions*, **2008**, 234-40	4.3	62
208	Two 3d-4f nanomagnets formed via a two-step in situ reaction of picolinaldehyde. *Chemical Communications*, **2013**, 49, 6549-51	5.8	61
207	Reversible chemisorption of sulfur dioxide in a spin crossover porous coordination polymer. *Inorganic Chemistry*, **2013**, 52, 12777-83	5.1	61
206	Theoretical search for new ferromagnetically coupled transition metal complexes. *Chemical Communications*, **1998**, 2767-2768	5.8	61

205	Structure and magnetism of dinuclear copper(II) metallacyclophanes with oligoacenebis(oxamate) bridging ligands: theoretical predictions on wirelike magnetic coupling. *Journal of the American Chemical Society*, **2008**, 130, 576-85	16.4	60
204	A molecular pair of [GdNi3] tetrahedra bridged by water molecules. *Chemistry - A European Journal*, **2011**, 17, 8264-8	4.8	57
203	Theoretical study of the exchange coupling in copper(II) binuclear compounds with oxamidate and related polyatomic bridging ligands *Journal of the Chemical Society Dalton Transactions*, **1999**, 1669-1676		57
202	Structures, magnetochemistry, spectroscopy, theoretical study, and catechol oxidase activity of dinuclear and dimer-of-dinuclear mixed-valence Mn(III)Mn(II) complexes derived from a macrocyclic ligand. *Inorganic Chemistry*, **2013**, 52, 7732-46	5.1	56
201	Copper(II) complexes with 4-amino-N-[4,6-dimethyl-2-pyrimidinyl]benzenesulfonamide. Synthesis, crystal structure, magnetic properties, EPR, and theoretical studies of a novel mixed mu-carboxylato, NCN-bridged dinuclear copper compound. *Inorganic Chemistry*, **2001**, 40, 3089-96	5.1	56
200	Molecules composed of two weakly magnetically coupled [MnIII4] clusters. *Inorganic Chemistry*, **2007**, 46, 9045-7	5.1	54
199	Increasing the effective energy barrier promoted by the change of a counteranion in a Zn-Dy-Zn SMM: slow relaxation via the second excited state. *Chemical Communications*, **2015**, 51, 12353-6	5.8	53
198	Exchange coupling in CuIIGdIII dinuclear complexes: A theoretical perspective. *Comptes Rendus Chimie*, **2008**, 11, 1227-1234	2.7	53
197	Single-molecule magnetism arising from cobalt(II) nodes of a crystalline sponge. *Journal of Materials Chemistry C*, **2017**, 5, 835-841	7.1	51
196	Magneto-structural correlation studies and theoretical calculations of a unique family of single end-to-end azide-bridged Ni(II)4 cyclic clusters. *Inorganic Chemistry*, **2010**, 49, 9517-26	5.1	51
195	A new family of oxime-based hexanuclear manganese(III) single molecule magnets with high anisotropy energy barriers. *Chemical Communications*, **2010**, 46, 5106-8	5.8	51
194	Electronic Structure and Magnetic Behavior in Polynuclear Transition-Metal Compounds227-279		51
193	Amending the anisotropy barrier and luminescence behavior of heterometallic trinuclear linear [M(II) -Ln(III) -M(II)] (Ln(III) =Gd, Tb, Dy; M(II) =Mg/Zn) complexes by change from divalent paramagnetic to diamagnetic metal ions. *Chemistry - A European Journal*, **2015**, 21, 6449-64	4.8	50
192	Modulation of single-molecule magnet behaviour via photochemical [2+2] cycloaddition. *Chemical Communications*, **2015**, 51, 15358-61	5.8	50
191	A family of ferro- and antiferromagnetically coupled decametallic chromium(III) wheels. *Chemistry - A European Journal*, **2006**, 12, 1385-96	4.8	50
190	First evidence of light-induced spin transition in molybdenum(IV). *Chemical Communications*, **2015**, 51, 8229-32	5.8	49
189	New oxamidato-bridged Cu(II)-Ni(II) complexes: supramolecular structures with thiocyanate ligands and hydrogen bonds. Magnetostructural studies: DFT calculations. *Inorganic Chemistry*, **2002**, 41, 6780-9	5.1	49
188	Further Theoretical Evidence for the Exceptionally Strong Ferromagnetic Coupling in Oxo-Bridged Cu(II) Dinuclear Complexes. *Journal of Physical Chemistry A*, **2002**, 106, 4938-4941	2.8	47

187	Guest modulation of spin-crossover transition temperature in a porous iron(II) metal-organic framework: experimental and periodic DFT studies. *Chemistry - A European Journal*, **2014**, 20, 12864-73	4.8	46
186	Interconversion of quadruply and quintuply bonded molybdenum complexes by reductive elimination and oxidative addition of dihydrogen. *Angewandte Chemie - International Edition*, **2013**, 52, 3227-31	16.4	45
185	Slow Magnetic Relaxation in a CoIIYIII Single-Ion Magnet with Positive Axial Zero-Field Splitting. *Angewandte Chemie*, **2013**, 125, 9300-9304	3.6	44
184	Reply to Comment on About the calculation of exchange coupling constants using density-functional theory: The role of the self-interaction error J. Chem. Phys. 123, 164110 (2005)]. *Journal of Chemical Physics*, **2006**, 124, 107102	3.9	44
183	Multiscale study of mononuclear Co SMMs based on curcuminoid ligands. *Chemical Science*, **2016**, 7, 2793-2803	9.4	43
182	2-Methyl-1-hexen-3-yne Lewis Base Stabilized Diketonate Copper(I) Complexes: X-ray Structures, Theoretical Study, and Low-Temperature Chemical Vapor Deposition of Copper Metal. *Chemistry of Materials*, **2001**, 13, 3993-4004	9.6	43
181	Magnetic bistability and thermochromism in a molecular Cu(II) chain. *Inorganic Chemistry*, **2009**, 48, 1269-71	5.1	42
180	Density functional study of exchange coupling constants in single-molecule magnets: the Fe8 complex. *Chemistry - A European Journal*, **2005**, 11, 4767-71	4.8	42
179	Exchange coupling constants using Density Functional Theory: long-range corrected functionals. *Journal of Computational Chemistry*, **2011**, 32, 1998-2004	3.5	41
178	Theoretical Study of the Magnetic Properties of an Mn12 Single-Molecule Magnet with a Loop Structure: The Role of the Next-Nearest Neighbor Interactions. *Journal of Chemical Theory and Computation*, **2007**, 3, 782-8	6.4	41
177	Theoretical study of exchange coupling constants in an Fe19 complex. *Journal of Physics and Chemistry of Solids*, **2004**, 65, 799-803	3.9	41
176	Room-temperature synthesis and crystal, magnetic, and electronic structure of the first silver copper oxide. *Inorganic Chemistry*, **2002**, 41, 6604-13	5.1	41
175	A Pseudo-Octahedral Cobalt(II) Complex with Bispyrazolylpyridine Ligands Acting as a Zero-Field Single-Molecule Magnet with Easy Axis Anisotropy. *Chemistry - A European Journal*, **2018**, 24, 8857-8868	4.8	40
174	Designing a Dy Single-Molecule Magnet with Two Well-Differentiated Relaxation Processes by Using a Nonsymmetric Bis-bidentate Bipyrimidine- N-Oxide Ligand: A Comparison with Mononuclear Counterparts. *Inorganic Chemistry*, **2018**, 57, 6362-6375	5.1	40
173	Analysis of Magnetic Anisotropy and the Role of Magnetic Dilution in Triggering Single-Molecule Magnet (SMM) Behavior in a Family of Co Y Dinuclear Complexes with Easy-Plane Anisotropy. *Chemistry - A European Journal*, **2017**, 23, 11649-11661	4.8	39
172	Theoretical determination of multiple exchange couplings and magnetic susceptibility data in inorganic solids: the prototypical case of Cu2(OH)3NO3. *Journal of Physical Chemistry B*, **2006**, 110, 115-8	3.4	39
171	Asymmetry and magnetism in bis(oximato)-bridged heterobimetallic compounds: a computational approach. *Chemistry - A European Journal*, **2000**, 6, 327-33	4.8	39
170	Electron transfer in the [Pt(NH3)4]2+ [W(CN)8]3- donor-acceptor system. The environment effect: a time-dependent density functional study. *Journal of the American Chemical Society*, **2001**, 123, 10742-3	16.4	39

169	Huge magnetic anisotropy in a trigonal-pyramidal nickel(II) complex. *Inorganic Chemistry*, **2014**, 53, 676-8	5.1	38
168	Effect of metal complexation on the conductance of single-molecular wires measured at room temperature. *Journal of the American Chemical Society*, **2014**, 136, 8314-22	16.4	38
167	Exchange interactions in azido-bridged ligand Ni(II) complexes: a theoretical analysis. *Inorganic Chemistry*, **2009**, 48, 3139-44	5.1	38
166	Ab initio study of the bare and hydrated (001) surface of tetragonal zirconia. *Surface Science*, **1992**, 275, 482-492	1.8	38
165	Investigation of easy-plane magnetic anisotropy in P-ligand square-pyramidal Co single ion magnets. *Chemical Communications*, **2017**, 53, 5338-5341	5.8	37
164	Spin dynamics in single-molecule magnets and molecular qubits. *Dalton Transactions*, **2020**, 49, 9916-9928	4.3	37
163	Lanthanide Tetrazolate Complexes Combining Single-Molecule Magnet and Luminescence Properties: The Effect of the Replacement of Tetrazolate N3 by β-Diketonate Ligands on the Anisotropy Energy Barrier. *Chemistry - A European Journal*, **2016**, 22, 14548-59	4.8	37
162	Sequential Electron Transport and Vibrational Excitations in an Organic Molecule Coupled to Few-Layer Graphene Electrodes. *ACS Nano*, **2016**, 10, 2521-7	16.7	36
161	Two C3 -symmetric Dy3III complexes with triple di-μ-methoxo-μ-phenoxo bridges, magnetic ground state, and single-molecule magnetic behavior. *Chemistry - A European Journal*, **2014**, 20, 8410-20	4.8	36
160	Magnetic coupling in trinuclear partial cubane copper(II) complexes with a hydroxo bridging core and peripheral phenoxo bridges from NNO donor Schiff base ligands. *Inorganica Chimica Acta*, **2010** , 363, 846-854	2.7	36
159	Mononuclear Fe(II) single-molecule magnets: a theoretical approach. *Inorganic Chemistry*, **2011**, 50, 4016-20	5.1	35
158	Early-late transition metal ferromagnetic coupling mediated by hydrogen bonding. *Chemical Communications*, **2002**, 2614-5	5.8	35
157	Six States Switching of Redox-Active Molecular Tweezers by Three Orthogonal Stimuli. *Journal of the American Chemical Society*, **2017**, 139, 9213-9220	16.4	34
156	Triangular nickel complexes derived from 2-pyridylcyanoxime: an approach to the magnetic properties of the [Ni3(μ3-OH){pyC(R)NO}3]2+ core. *Chemistry - A European Journal*, **2012**, 18, 3637-48	4.8	34
155	Synthesis, crystal structure and magnetic properties of two oxalato-bridged dimetallic trinuclear complexes combined with a polar cation. *Dalton Transactions*, **2010**, 39, 4951-8	4.3	34
154	A Theoretical Study of the Exchange Coupling in Hydroxo- and Alkoxo-Bridged Dinuclear Oxovanadium(IV) Compounds. *European Journal of Inorganic Chemistry*, **2004**, 2004, 143-153	2.3	34
153	Spin densities in a ferromagnetic bimetallic chain compound: polarized neutron diffraction and DFT calculations. *Journal of the American Chemical Society*, **2002**, 124, 14433-41	16.4	34
152	Ferro- to antiferromagnetic crossover angle in diphenoxido- and carboxylato-bridged trinuclear Ni(II)Mn(II) complexes: experimental observations and theoretical rationalization. *Inorganic Chemistry*, **2014**, 53, 9296-305	5.1	33

151	Synthesis, crystal structure and magnetism of new salicylamidoxime-based hexanuclear manganese(III) single-molecule magnets. *Dalton Transactions*, **2012**, 41, 13668-81	4.3	33
150	Exchange coupling constants using density functional theory: The M0X suite. *Chemical Physics Letters*, **2008**, 460, 336-338	2.5	33
149	Synthesis of a novel heptacoordinated Fe(III) dinuclear complex: experimental and theoretical study of the magnetic properties. *Dalton Transactions*, **2010**, 39, 4874-81	4.3	32
148	Structure, magnetic properties, polarized neutron diffraction, and theoretical study of a copper(II) cubane. *Chemistry - A European Journal*, **2008**, 14, 9540-8	4.8	32
147	Crystal Orbital Displacement Analysis of Interactions in the Solid State. Application to the Study of Host-Guest Interactions in the Hofmann Clathrates. *Journal of the American Chemical Society*, **1994**, 116, 8207-8221	16.4	32
146	Self-assembly of pentanuclear mesocate versus octanuclear helicate: size effect of the [M(II)3(μ3-O/X)]n+ triangle core. *Inorganic Chemistry*, **2013**, 52, 1099-107	5.1	31
145	Neutron diffraction and theoretical DFT studies of two dimensional molecular-based magnet K2[Mn(H2O)2]3[Mo(CN)7]2.6H2O. *Inorganic Chemistry*, **2007**, 46, 1090-9	5.1	31
144	Unprecedented ferromagnetic dipolar interaction in a dinuclear holmium(III) complex: a combined experimental and theoretical study. *Chemical Communications*, **2013**, 49, 9341-3	5.8	30
143	Magnetic properties of largest-spin single molecule magnets: Mn17 complexes--a density functional theory approach. *Inorganic Chemistry*, **2010**, 49, 9641-8	5.1	30
142	Experimental and theoretical studies on arene-bridged metal-metal-bonded dimolybdenum complexes. *Chemistry - A European Journal*, **2014**, 20, 6092-102	4.8	29
141	Slow relaxation of magnetization in a bis-mer-tridentate octahedral Co(ii) complex. *Dalton Transactions*, **2018**, 47, 859-867	4.3	29
140	Neodymium 1D systems: targeting new sources for field-induced slow magnetization relaxation. *Dalton Transactions*, **2015**, 44, 15774-8	4.3	27
139	Self-Assembly of Heterometallic Metallomacrocycles via Ditopic Fluoroaryl Gold(I) Organometallic Metalloligands. *Organometallics*, **2012**, 31, 1533-1545	3.8	27
138	Discovering the complex chemistry of a simple Ni(II)/H(3)L system: magnetostructural characterization and DFT calculations of Di- and polynuclear nickel(II) compounds. *Inorganic Chemistry*, **2009**, 48, 9861-73	5.1	27
137	Tailor-made strong exchange magnetic coupling through very long bridging ligands: theoretical predictions. *Inorganic Chemistry*, **2003**, 42, 4881-4	5.1	27
136	Electronic Structure and Bonding in CaC2. *The Journal of Physical Chemistry*, **1995**, 99, 3114-3119		27
135	Metal-Controlled Magnetoresistance at Room Temperature in Single-Molecule Devices. *Journal of the American Chemical Society*, **2017**, 139, 5768-5778	16.4	26
134	Design of dinuclear copper species with carboranylcarboxylate ligands: study of their steric and electronic effects. *Chemistry - A European Journal*, **2011**, 17, 13217-29	4.8	26

133	Strong magnetic interactions through weak bonding interactions in organometallic radicals: combined experimental and theoretical study. *Chemistry - A European Journal*, **2007**, 13, 8858-66	4.8	26
132	Quantitative Estimation of Ising-Type Magnetic Anisotropy in a Family of C -Symmetric Co Complexes. *Chemistry - A European Journal*, **2017**, 23, 12550-12558	4.8	25
131	Theoretical modeling of two-step spin-crossover transitions in FeII dinuclear systems. *Journal of Materials Chemistry C*, **2015**, 3, 7954-7961	7.1	25
130	Squarato-metal(II) complexes. 2. unusual bonding mode for a squarato-bridged trinuclear copper(II) complex. *Inorganic Chemistry*, **2008**, 47, 4648-55	5.1	25
129	Magneto-Structural Correlations in Trinuclear Cu(II) Complexes: A Density Functional Study. *Monatshefte F□ Chemie*, **2003**, 134, 307-316	1.4	25
128	An Unprecedented Stimuli-Controlled Single-Crystal Reversible Phase Transition of a Metal-Organic Framework and Its Application to a Novel Method of Guest Encapsulation. *Advanced Materials*, **2018**, 30, e1800726	24	25
127	Charge transfer and tunable ambipolar effect induced by assembly of Cu(II) binuclear complexes on carbon nanotube field effect transistor devices. *Journal of the American Chemical Society*, **2012**, 134, 7896-901	16.4	24
126	S(T) = 22 [Mn10] supertetrahedral building-block to design extended magnetic networks. *Inorganic Chemistry*, **2011**, 50, 8580-7	5.1	24
125	CoIILnIII dinuclear complexes (LnIII = Gd, Tb, Dy, Ho and Er) as platforms for 1,5-dicyanamide-bridged tetranuclear CoII2LnIII2 complexes: A magneto-structural and theoretical study. *Comptes Rendus Chimie*, **2012**, 15, 878-888	2.7	23
124	Rational Design of Lanthanoid Single-Ion Magnets: Predictive Power of the Theoretical Models. *Chemistry - A European Journal*, **2016**, 22, 13532-9	4.8	22
123	Theoretical Modeling of the Ligand-Tuning Effect over the Transition Temperature in Four-Coordinated Fe(II) Molecules. *Inorganic Chemistry*, **2016**, 55, 1657-63	5.1	22
122	Spin-crossover behavior in two new supramolecular isomers. *Inorganic Chemistry*, **2014**, 53, 201-8	5.1	22
121	Interconversion of Quadruply and Quintuply Bonded Molybdenum Complexes by Reductive Elimination and Oxidative Addition of Dihydrogen. *Angewandte Chemie*, **2013**, 125, 3309-3313	3.6	22
120	Can theoretical methods go beyond the experimental data? The case of molecular magnetism. *Dalton Transactions*, **2009**, 5873-8	4.3	22
119	Magnetic exchange interaction in triply bridged dinickel(II) complexes. *Chemical Physics Letters*, **2008**, 452, 38-43	2.5	22
118	Exchange coupling mediated by N-H□□Cl hydrogen bonds: experimental and theoretical study of the frustrated magnetic system in bis(o-phenylenediamine)nickel(II) chloride. *Inorganic Chemistry*, **2012**, 51, 5487-93	5.1	21
117	The use of a bis(phenylpyrazolyl)pyridyl ligand to prepare [Mn4] and [Mn10] cage complexes. *Chemistry - A European Journal*, **2011**, 17, 4960-3	4.8	21
116	Theoretical study of the exchange coupling in a Ni12 single-molecule magnet. *Dalton Transactions*, **2006**, 2643-6	4.3	21

115	Theoretical clues to the mechanism of dioxygen formation at the oxygen-evolving complex of photosystem II. *Chemistry - A European Journal*, **2002**, 8, 2508-15	4.8	21
114	Exchange Coupling in Metal Complexes of the Second Transition Series: A Theoretical Exploration. *European Journal of Inorganic Chemistry*, **2003**, 2003, 1756-1760	2.3	21
113	Theoretical determination of the exchange coupling constants of a single-molecule magnet Fe10 complex. *Chemical Physics Letters*, **2005**, 415, 6-9	2.5	21
112	Control over Near-Ballistic Electron Transport through Formation of Parallel Pathways in a Single-Molecule Wire. *Journal of the American Chemical Society*, **2019**, 141, 240-250	16.4	20
111	Strong Antiferromagnetic Coupling at Long Distance through a Ligand to Metal Charge Transfer Mechanism. *Journal of Physical Chemistry C*, **2007**, 111, 618-621	3.8	19
110	Single-ion magnetic anisotropy in a vacant octahedral Co(ii) complex. *Dalton Transactions*, **2018**, 48, 25-29	4.3	19
109	A racemic and enantiopure unsymmetric diiron(III) complex with a chiral o-carborane-based pyridylalcohol ligand: combined chiroptical, magnetic, and nonlinear optical properties. *Chemistry - A European Journal*, **2014**, 20, 1081-90	4.8	18
108	Hexanuclear copper(II) cages built on a central {□-O□□H□□□-O} moiety, 1,3-bis(dimethylamino)-2-propanolato and capping R-phosphonates: crystal structures, magnetic behavior, and DFT studies. *Inorganic Chemistry*, **2012**, 51, 6842-50	5.1	18
107	Magnetic interactions mediated by diamagnetic cations in [Mn18M] (M = Sr2+, Y3+, Cd2+, and Lu3+) coordination clusters. *Inorganic Chemistry*, **2013**, 52, 5764-74	5.1	18
106	Encouraging Chromium(III) Ions to Form Larger Clusters: Syntheses, Structures, Magnetic Properties and Theoretical Studies of Di- and Octametallic Cr Clusters. *European Journal of Inorganic Chemistry*, **2006**, 2006, 3382-3392	2.3	18
105	Exchange coupling in mu-aqua:mu-oxo vs. di-mu-hydroxo dinuclear Cu(II) compounds: a density functional study. *Dalton Transactions*, **2005**, 2624-9	4.3	18
104	Dendrimers Containing Two Metallic Layers. Chloride Migration from Peripheral Gold, Palladium, or Rhodium Metals to Internal Ruthenium Atoms. *Organometallics*, **2005**, 24, 6365-6373	3.8	18
103	A novel hexanuclear mixed oxidation state Cu(II)(4)Cu(I)(2) cluster complex exhibiting weak ferromagnetic exchange. *Inorganic Chemistry*, **2003**, 42, 1107-11	5.1	18
102	Theoretical study of the magnetic behavior of ferric wheels. *ChemPhysChem*, **2005**, 6, 1094-9	3.2	18
101	Electronic Structure of Host Lattices for Intercalation Compounds: SnS2, SnSe2, ZrS2, and TaS2. *Chemistry of Materials*, **1998**, 10, 3422-3428	9.6	18
100	Single-Molecule Magnet Properties of Transition-Metal Ions Encapsulated in Lacunary Polyoxometalates: A Theoretical Study. *Inorganic Chemistry*, **2016**, 55, 6405-13	5.1	17
99	A MnII6MnIII6 single-strand molecular wheel with a reuleaux triangular topology: synthesis, structure, magnetism, and DFT studies. *Inorganic Chemistry*, **2013**, 52, 12070-9	5.1	17
98	A mixed-valent pentanuclear Cu(II)(4)Cu(I) compound containing a radical-anion ligand. *Inorganic Chemistry*, **2009**, 48, 10643-51	5.1	17

97	Electronic Interactions in (η6-Arene) Ferracarboranes1. *Organometallics*, **2002**, 21, 4129-4137	3.8	17
96	Host.cntdot..cntdot..cntdot.Guest Interactions in the Pyrrole and Aniline Hofmann Clathrates. A Theoretical Study. *Inorganic Chemistry*, **1995**, 34, 3260-3269	5.1	17
95	Ab Initio Study of the Intermolecular Interactions in the Hofmann Clathrates. *The Journal of Physical Chemistry*, **1995**, 99, 2296-2306		17
94	Spin-polarized transport through single-molecule magnet Mn6 complexes. *Nanoscale*, **2013**, 5, 4751-7	7.7	16
93	Negatively charged metallacarborane redox couples with both members stable to air. *Chemistry - A European Journal*, **2015**, 21, 6888-97	4.8	16
92	Thermal behavior of Si-doped fullerenes vs their structural stability at T=0K: A density functional study. *Chemical Physics Letters*, **2011**, 510, 14-17	2.5	16
91	All-round robustness of the Mn19 coordination cluster system: experimental validation of a theoretical prediction. *Chemical Communications*, **2014**, 50, 5847-50	5.8	15
90	Magnetic communication through functionalized nanotubes: a theoretical study. *Nano Letters*, **2006**, 6, 380-4	11.5	15
89	Symmetry and Topology Determine the MoVCNMnII Exchange Interactions in High-Spin Molecules. *Angewandte Chemie*, **2005**, 117, 2771-2775	3.6	15
88	Ferromagnetic interaction in mu1,3-cyanamido-derived copper(II) cryptates. *Chemistry - A European Journal*, **2004**, 11, 398-405	4.8	15
87	Theoretical approach to the magnetostructural correlations in the spin-Peierls compound CuGeO3. *Physical Review B*, **2000**, 61, 54-57	3.3	15
86	Mononuclear Lanthanide Complexes with 18-Crown-6 Ether: Synthesis, Characterization, Magnetic Properties, and Theoretical Studies. *Inorganic Chemistry*, **2018**, 57, 13225-13234	5.1	15
85	Computational Modeling of Transition Temperatures in Spin-Crossover Systems. *Comments on Inorganic Chemistry*, **2019**, 39, 216-241	3.9	14
84	Fatty acid carboxylate- and anionic surfactant-controlled delivery systems that use mesoporous silica supports. *Chemistry - A European Journal*, **2010**, 16, 10048-61	4.8	14
83	Electronic and Steric Control of the Spin-Crossover Behavior in [(Cp)Mn] Manganocenes. *Inorganic Chemistry*, **2018**, 57, 702-709	5.1	13
82	Electronic Structure Modulation in an Exceptionally Stable Non-Heme Nitrosyl Iron(II) Spin-Crossover Complex. *Chemistry - A European Journal*, **2016**, 22, 12741-51	4.8	13
81	Single-molecule magnet Fe9 supramolecular dimers: a theoretical approach to intramolecular and intermolecular exchange interactions. *Chemical Communications*, **2009**, 4363-5	5.8	13
80	Localized Orbitals vs. Pseudopotential-Plane Waves Basis Sets: Performances and Accuracy for Molecular Magnetic Systems. *Monatshefte Fü Chemie*, **2003**, 134, 317-326	1.4	13

79	Unprecedented trimetallic cluster with an in-plane .mu.3-hydride ligand. X-ray crystal structure of [Mo2(CO)8(.mu.-dppm)(.mu.3-H)(.mu.-AuPPh3)]. *Organometallics*, **1992**, 11, 3753-3759	3.8	13
78	Effect of Heteroatoms on Field-Induced Slow Magnetic Relaxation of Mononuclear Fe (S = 5/2) Ions within Polyoxometalates. *Inorganic Chemistry*, **2018**, 57, 6957-6964	5.1	13
77	Magnetization Slow Dynamics in Ferrocenium Complexes. *Chemistry - A European Journal*, **2019**, 25, 10625-10632	5.2	12
76	Exchange Interactions on the Highest-Spin Reported Molecule: the Mixed-Valence Fe42 Complex. *Scientific Reports*, **2016**, 6, 23847	4.9	12
75	Electric-field induced bistability in single-molecule conductance measurements for boron coordinated curcuminoid compounds. *Chemical Science*, **2018**, 9, 6988-6996	9.4	12
74	Antiferromagnetism or delocalized spin in a Cu3S2 core?. *Chemistry - A European Journal*, **2010**, 16, 2726-38	5.2	12
73	Electronic Structure and Dynamic Properties of Solid Alkali Cyanides. *Journal of Physical Chemistry A*, **1997**, 101, 1393-1399	2.8	12
72	Coming full circle: constructing a [Gd] wheel dimer by dimer and the importance of spin topology. *Dalton Transactions*, **2017**, 46, 10255-10263	4.3	11
71	Tuning Single-Molecule Conductance in Metalloporphyrin-Based Wires via Supramolecular Interactions. *Angewandte Chemie - International Edition*, **2020**, 59, 19193-19201	16.4	11
70	Antiferro- to ferromagnetic crossover in diphenoxido bridged NiII2MnII complexes derived from N2O2 donor Schiff base ligands. *Polyhedron*, **2016**, 117, 57-63	2.7	11
69	Slow-spin relaxation of a low-spin S = 1/2 Fe carborane complex. *Chemical Communications*, **2019**, 55, 3825-3828	5.8	10
68	Pyridinethiolate Titanocene Metalloligands and Their Self-Assembly Reactions To Yield Early□late Metallamacrocycles. *Organometallics*, **2016**, 35, 336-345	3.8	10
67	Tunable Magnetization Dynamics through Solid-State Ligand Substitution Reaction. *Inorganic Chemistry*, **2017**, 56, 8829-8836	5.1	10
66	Structure of the non-polar (101 0) surfaces of AlN and □SiC: a periodic Hartree-Fock study. *Surface Science*, **1996**, 355, 167-176	1.8	10
65	Room temperature conductance switching in a molecular iron(iii) spin crossover junction. *Chemical Science*, **2020**, 12, 2381-2388	9.4	10
64	Antiferromagnetic Interactions in Copper(II) □-Oxalato Dinuclear Complexes: The Role of the Counterion. *European Journal of Inorganic Chemistry*, **2018**, 2018, 509-516	2.3	9
63	Structure, magnetic properties and DFT calculations of azido-copper(II) complexes with different azido-bonding, nuclearity and dimensionality. *New Journal of Chemistry*, **2018**, 42, 2627-2639	3.6	9
62	Predetermined Ferromagnetic Coupling via Strict Control of M-O-M Angles. *Inorganic Chemistry*, **2016**, 55, 11707-11715	5.1	9

61	Ni-2,3-thiophenedithiolate Anions in New Architectures: An In-Line Mixed-Valence Ni Dithiolene (Ni4S12) Cluster. *European Journal of Inorganic Chemistry*, **2011**, 2011, 4807-4815	2.3	9
60	Theoretical Study of Host.cntdot..cntdot..cntdot.Guest Interactions in Clathrates with a Cd(CN)2 Host. *Inorganic Chemistry*, **1995**, 34, 5845-5851	5.1	9
59	A trinuclear Cu(II) complex with functionalized s-heptazine N-ligands: molecular chemistry from a g-C3N4 fragment. *Dalton Transactions*, **2015**, 44, 15761-3	4.3	8
58	MEPROCS framework for Craniofacial Superimposition: Validation study. *Legal Medicine*, **2016**, 23, 99-108	1.9	8
57	An Unsaturated Four-Coordinate Dimethyl Dimolybdenum Complex with a Molybdenum-Molybdenum Quadruple Bond. *Chemistry - A European Journal*, **2017**, 23, 194-205	4.8	8
56	Theoretical study of the electronic properties and exchange coupling in a Ni4 cubane like single-molecule magnet. *Physica B: Condensed Matter*, **2006**, 384, 123-125	2.8	8
55	An Fe11 complex showing single-molecule magnet behavior: Theoretical study using density functional methods and Monte Carlo simulations. *Polyhedron*, **2005**, 24, 2364-2367	2.7	8
54	Ferromagnetism in polynuclear systems based on non-linear [MnII2MnIII] building blocks. *Inorganic Chemistry Frontiers*, **2016**, 3, 1272-1279	6.8	7
53	Experimental and theoretical study of the spin ground state of the high-spin molecular cluster [NiII{NiII(CH3OH)3}8(□CN)30{WV(CN)3}6]□15CH3OH by polarised neutron diffraction and density functional theory calculations. *Inorganica Chimica Acta*, **2008**, 361, 3609-3615	2.7	7
52	Exchange coupling interactions in a Fe6 complex: A theoretical study using density functional theory. *Physica B: Condensed Matter*, **2006**, 384, 116-119	2.8	7
51	Ab initio study of AlN and alpha -SiC (112-bar0) surface relaxation. *Physical Review B*, **1996**, 53, 4933-4938	3.3	7
50	Assessment of the SCAN Functional for Spin-State Energies in Spin-Crossover Systems. *Journal of Physical Chemistry A*, **2020**, 124, 5053-5058	2.8	7
49	Different topologies in three manganese-□azido 1D compounds: magnetic behavior and DFT-quantum Monte Carlo calculations. *Dalton Transactions*, **2015**, 44, 18632-42	4.3	6
48	DFT approaches to transport calculations in magnetic single-molecule devices. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	6
47	Magnetic and transport properties of Fe single-molecule magnets: a theoretical insight. *Dalton Transactions*, **2016**, 45, 18867-18875	4.3	6
46	Boosting Self-Assembly Diversity in the Solid-State by Chiral/Non-Chiral Zn -Porphyrin Crystallization. *Chemistry - A European Journal*, **2018**, 24, 12950-12960	4.8	6
45	Exchange Coupling in Di- and Polynuclear Complexes **2013**, 501-549		6
44	Exchange coupling and magnetic anisotropy of exchanged-biased quantum tunnelling single-molecule magnet Ni3Mn2 complexes using theoretical methods based on Density Functional Theory. *Dalton Transactions*, **2012**, 41, 2659-66	4.3	6

43	Spins on a curved surface: an Fe(III)14 ferracalixarene. *Dalton Transactions*, **2013**, 42, 9606-12	4.3	6
42	Extended Fe butterfly complexes: theoretical analysis of magnetic properties and magnetostructural maps. *Dalton Transactions*, **2010**, 39, 4832-7	4.3	6
41	Dinuclear CoYvs. tetranuclear CoY complexes: the effect of increasing molecular size on magnetic anisotropy and relaxation dynamics. *Dalton Transactions*, **2019**, 48, 14873-14884	4.3	5
40	Dysprosium-based complexes with a flat pentadentate donor: a magnetic and ab initio study. *Dalton Transactions*, **2020**, 49, 8389-8401	4.3	5
39	Element-Selective Molecular Charge Transport Characteristics of Binuclear Copper(II)-Lanthanide(III) Complexes. *Inorganic Chemistry*, **2018**, 57, 9274-9285	5.1	5
38	Theoretical study of the exchange coupling interactions in a polyoxometalate Fe9W12 complex. *Polyhedron*, **2007**, 26, 2161-2164	2.7	5
37	Exchange interactions in a Fe5 complex: A theoretical study using density functional theory. *Inorganica Chimica Acta*, **2008**, 361, 3832-3835	2.7	5
36	Cation templation of Mn2+/[Mo(CN)7]4 system: Formation of pseudo-dimorphs (NH4)2Mn3(H2O)4[Mo(CN)7]2 nH2O (n = 4, 5). *Polyhedron*, **2005**, 24, 1033-1046	2.7	5
35	Theoretical study of the guest?guest interactions of cobaltocene intercalated in metal sulfides. *Dalton Transactions RSC*, **2000**, 1463-1467		5
34	Electronic structure and properties of hexagonal wurtzite-type SiC. *International Journal of Quantum Chemistry*, **1994**, 52, 365-373	2.1	5
33	Room-Temperature Spin-Dependent Transport in Metalloporphyrin-Based Supramolecular Wires. *Angewandte Chemie - International Edition*, **2021**, 60, 25958-25965	16.4	5
32	Single-Molecule Transport of Fullerene-Based Curcuminoids. *Journal of Physical Chemistry C*, **2020**, 124, 2698-2704	3.8	5
31	Slow magnetic relaxation in dinuclear dysprosium and holmium phenoxide bridged complexes: a Dy2 single molecule magnet with a high energy barrier. *Inorganic Chemistry Frontiers*, **2021**, 8, 2532-2541	6.8	5
30	Electronic Structure and Magnetic Behavior in Polynuclear Transition-Metal Compounds227-279		5
29	Models to predict the magnetic properties of single- and multiple-bridged phosphate CuII systems: a theoretical DFT insight. *Inorganic Chemistry Frontiers*, **2017**, 4, 509-520	6.8	4
28	One-Dimensional Intercalation Compound 2 HgS?SnBr2: Ab Initio Electronic Structure Calculations and Molecular Dynamics Simulations. *Chemistry - A European Journal*, **1998**, 4, 2485-2492	4.8	4
27	Theoretical study of the intercalation of cobaltocene in metal chalcogenides. *Journal of Materials Chemistry*, **1998**, 8, 1893-1900		4
26	[UF] : A Molecular Hexafluorido Actinide(IV) Complex with Compensating Spin and Orbital Magnetic Moments. *Angewandte Chemie - International Edition*, **2019**, 58, 15650-15654	16.4	3

25	Electronic structure and localization properties of C60Tan clusters (n=1,3): A first-principles study. *Physical Review B*, **2010**, 81,	3.3	3
24	Room-Temperature Spin-Dependent Transport in Metalloporphyrin-Based Supramolecular Wires. *Angewandte Chemie*, **2021**, 133, 26162	3.6	3
23	Tuning Single-Molecule Conductance in Metalloporphyrin-Based Wires via Supramolecular Interactions. *Angewandte Chemie*, **2020**, 132, 19355-19363	3.6	3
22	Experimental and Computational Studies on Quadruply Bonded Dimolybdenum Complexes with Terminal and Bridging Hydride Ligands. *Chemistry - A European Journal*, **2021**, 27, 6569-6578	4.8	3
21	Self-Assembled, Highly Positively Charged, Allyl-Pd Crowns: Cavity-Pocket-Driven Interactions of Fluoroanions. *Chemistry - A European Journal*, **2020**, 26, 7847-7860	4.8	2
20	Influence of the Disposition of the Anisotropy Axes into the Magnetic Properties of Mn Dinuclear Compounds with Benzoato Derivative Bridges. *Inorganic Chemistry*, **2017**, 56, 8135-8146	5.1	2
19	Magnetic Behaviour of Transition Metal Complexes with Functionalized Chiral and C60-Filled Nanotubes as Bridging Ligands: A Theoretical Study. *Magnetochemistry*, **2015**, 1, 62-71	3.1	2
18	The dilemma of CrIIINiII exchange interactions: ferromagnetism versus antiferromagnetism. *Chemistry - A European Journal*, **2011**, 17, 8841-9	4.8	2
17	Intercalation of Halogen Molecules in Alkali Fluoride Lattices: A Theoretical Study. *Journal of the American Chemical Society*, **1995**, 117, 2877-2883	16.4	2
16	Modeling Magnetic Properties with Density Functional Theory-Based Methods **2016**, 419-446		1
15	A density functional theory approach to the magnetic properties of a coupled single-molecule magnet (Mn7)2 complex An entangled qubit pair candidate. *Canadian Journal of Chemistry*, **2013**, 91, 866-871	0.9	1
14	Self-Assembly of Coordination Compounds: Design Principles **2012**,		1
13	Room-Temperature Synthesis and Crystal, Magnetic, and Electronic Structure of the First Silver Copper Oxide.. *ChemInform*, **2003**, 34, no		1
12	Density Functional Theory: Improving the Functionals, Extending the Applications **1996**, 359-394		1
11	Magnetic anisotropy in Yb complex candidates for molecular qubits: a theoretical analysis. *Physical Chemistry Chemical Physics*, **2021**, 23, 1976-1983	3.6	1
10	Spin-Phonon Coupling and Slow-Magnetic Relaxation in Pristine Ferrocenium. *Chemistry - A European Journal*, **2021**, 27, 16440-16447	4.8	1
9	Nickel(II) salicylaldiminates: Re-visiting a classic. *Polyhedron*, **2021**, 205, 115321	2.7	0
8	[Co/Fe(Alkyl-tpdt)]: Alkyl-Substituted Cobalt and Iron Bis-dithiolenethiophenic Complexes. *Inorganic Chemistry*, **2020**, 59, 9261-9269	5.1	

List of Publications

7	H-Mediated Magnetic Interactions between Layers in a 2D MnIIDicyanamide Polymer: Neutron Diffraction, DFT, and Quantum Monte Carlo Calculations. *European Journal of Inorganic Chemistry*, **2018**, 2018, 278-288	2.3
6	[UF6]2A Molecular Hexafluorido Actinide(IV) Complex with Compensating Spin and Orbital Magnetic Moments. *Angewandte Chemie*, **2019**, 131, 15797-15801	3.6
5	Rktitelbild: [UF6]2A Molecular Hexafluorido Actinide(IV) Complex with Compensating Spin and Orbital Magnetic Moments (Angew. Chem. 44/2019). *Angewandte Chemie*, **2019**, 131, 16084-16084	3.6
4	The coloring problem in Ba2Cu3VS6. *Dalton Transactions RSC*, **2000**, 1009-1011	
3	Localized Orbitals vs. Pseudopotential-Plane Waves Basis Sets: Performances and Accuracy for Molecular Magnetic Systems **2002**, 201-210	
2	Magneto-Structural Correlations in Trinuclear Cu(II) Complexes: A Density Functional Study **2003**, 191-200	
1	Metal-Organic Nanocapsules with Functionalized s-Heptazine Ligands. *Inorganic Chemistry*, **2021**, 60, 570-573	5.1